

Ethyl heptanoate
106-30-9 | DTXSID1040112

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.56

Global applicability domain: Inside

Local applicability domain index: 6.12e-01

Confidence level: 7.18e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptyl acetate</div> <div>Measured: 3.46</div> <div>Predicted: 3.40</div>	<div>Image not found</div> <div>Methyl n-nonanoate</div> <div>Measured: 4.32</div> <div>Predicted: 4.23</div>	<div>Image not found</div> <div>5-Nonanone</div> <div>Measured: 2.88</div> <div>Predicted: 3.11</div>
<div>Image not found</div> <div>Hexyl acrylate</div> <div>Measured: 3.33</div> <div>Predicted: 3.18</div>	<div>Image not found</div> <div>(3R)-3,7-Dimethyloct-6-enal</div> <div>Measured: 3.83</div> <div>Predicted: 3.59</div>	